Semiconductor Optoelectronics
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Lecture - 6
Density of States in a Quantum Well Structure

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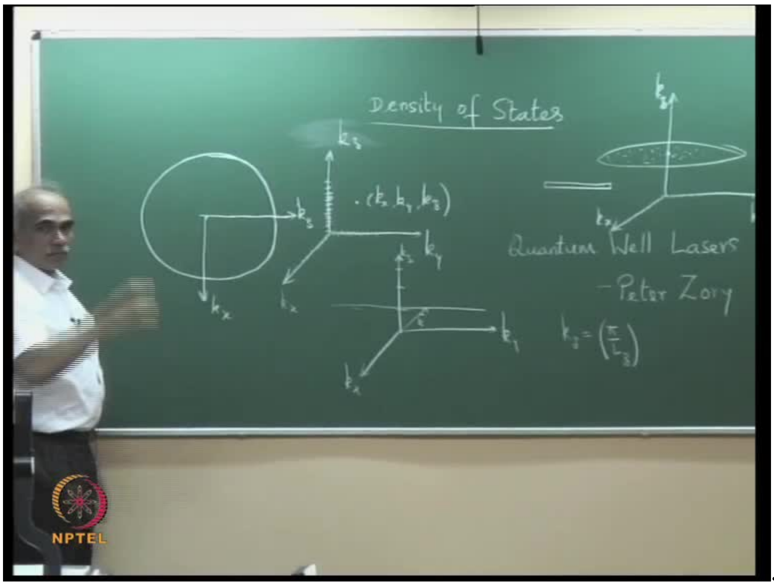

So, we continue with the density of states discussion and density of states in a quantum well structure. In the last class, we have discussed density of states for bulk semiconductors; and in the k space, in the k space I had shown that if this is k x, k y and k z; then in the k space, the k components can take very large number of values in general for a bulk semiconductor and therefore, the density of states available density of states is very large. And if you every point in the k space corresponding to a k x, k y, k z represents this state, then we have very large number of such states. But if I reduce the dimension of the semiconductor in one direction, let us say I reduce the dimension in the z direction to make it into a thin sheet, then correspondingly the density of states change. And what we have is k x and k y still are in very large number of values, however the allowed values for k z become highly discretised.

And since every k must have these three components; in this sheet an electron wave propagating through the sheet has to have three components of this; the first component of k non zero component of k z is here. So this is k z is here, which means every k value that you can think of must have one value k z here, which means the tip of the k vector, the tip of the k vector in the k space must lie on a plane k z equal to constant. So for the first value k z equal to constant is simply k z equal to pi by L z into m equal to 1, q equal to 1. So k z the first value is pi by L z therefore, all points the vector k can take large number of values still, but the tip of the vector must lie in this plane.

Therefore, in calculating the density of states, so we had this picture here, where this is k z, k z, k x and k y we considered discs with k z equal to constant, the first one. And in this because k x and k y take very large number of values or permitted to take large number of values corresponding to each k x and k y, we have a point a permitted point in this disc, which means if I slip the disc and show the disc like this k z is here central axis k z; this is k x and this is k y.

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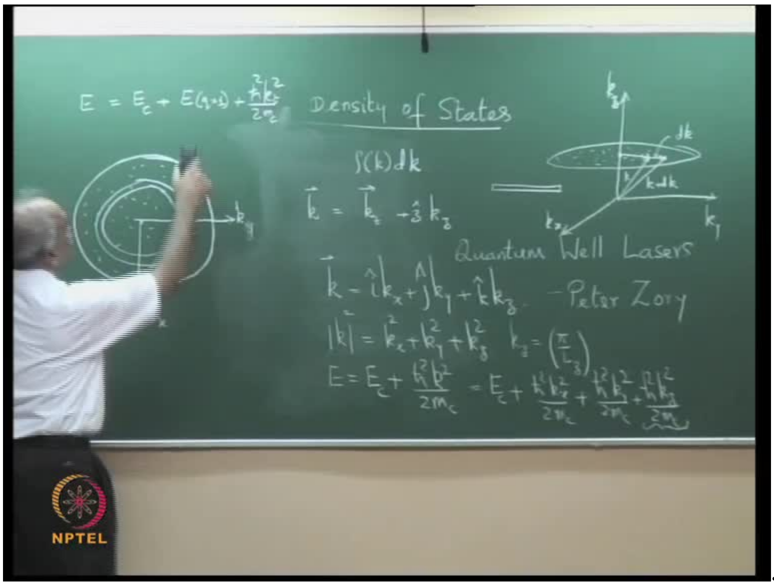

So, k x, k y and k z, k x, k x, k y, k z that is this disc in the k space I am showing like this, so k z is coming up k x, k y, k z in this you see large number of allowed values. Our objective is to find out rho of k which is defined through rho of k d k is the number of number of states between k and k plus d k, so if this is some value k and the next value k plus d k if it stands here, so this is k, this is k plus d k which means this is the vector d k here, this is d k then our objective is to find the number of allowed states between k and k plus d k if you see in this the k will correspond to a value which is here please see this is the disk the k can take any value like this between k and k plus d k.

So, this will correspond to a circle here a circle corresponding to k and the next circle outside corresponding to k plus d k, this transverse component here you see k is equal to i k x unit vector i plus, j unit vector k y, k y plus unit vector k into k z and mod k square that is k square is equal to k x square plus k y square plus k z square, we have energy E is equal to E c plus h cross square, k square divided by twice m c, which I can write as E c plus, for this disc q is equal to 1 the first value of k z corresponds to q equal to 1 therefore, I write this as h cross square, k x square by 2 m c I am just substituting this and h cross square k 1 square by 2 m c plus h cross square k z square by 2 m c, the vector here this vector k I can write as k equal to this is the vector i cap k x plus j cap k y I can write this as a transverse vector k t, this is the transverse vector on this plane without the z component plus z cap into k z, this is the transverse vector plus z cap into k z the complete vector. So, this part here k x square plus k y square I can call it as k t square and I write the energy E is equal to E c plus E of q equal to 1 plus h cross square k t square by 2 m c where E of q equal to 1 is this component h cross square k z square by 2 m c if i put q equal to 1 k z takes the value k z is equal to pi by L z.

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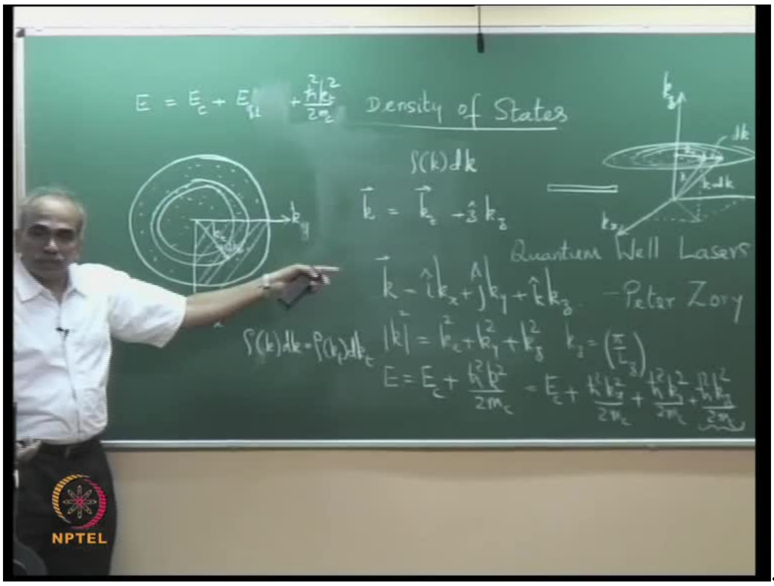

So, I can write this as E c plus E at q equal to 1 this E stands for that component only here or sometimes it is denoted as E q 1 either you can write this as E c, E at q equal to 1 or E q 1 plus h cross square k t square by 2 m c our objective is to find the number of points in this plane, so this is k t and this additional vector here is d k t please see here this is k, this is k plus d k corresponding to k there is a k t which has only 2 components x component and y component you can just drop down here and you find out what is the x component what is the y component and this is the z component, so what is k t? k t is just this that vector which has x component and y component do you follow, so it is these 2 components make this transverse vector, so this you see if I drop from here that is k t and d k t is the incremental volume, incremental vector, so that is d k t. So we have to find out the number of points therefore, the number of points between k and k plus d k is the same as number of points between k t and k t plus d k t do you agree because k can sit anywhere around this circle and k plus d k can sit anywhere here the number of points is the same between k and k plus d k in fact it is rho k, rho of k, d k is equal to rho of k t, d k t the number of points as for as the number of points is concerned it is the same.

So, to find out the number points, point means every point represents an allowed state number of points between k and d k plus and remember we have to take only the positive k x, positive k y and positive k z values because the negative values are already taken into account in our boundary condition. And therefore, I need to consider only this quadrant, positive quadrant like in the case of the sphere I have to consider only the octant, positive octant.

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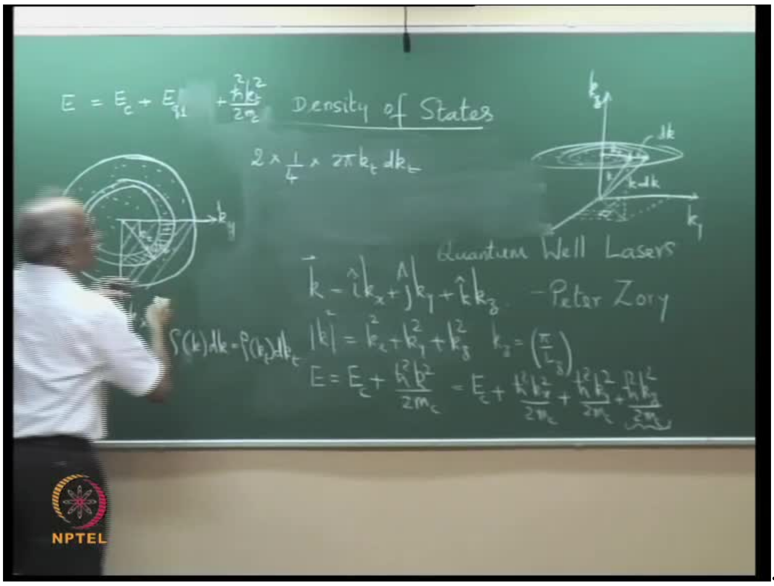

So, here of this circle I need to consider only the quadrant and therefore, what is the density of h the number of points always remember it has to come from definitions the number of points between k and k plus d k is in the positive octant or quadrant. So one forth into what is the number of points to find out the number of points I have to find out the area here now it is disc not the sphere in sphere what did we do we found out the volume between that shell and then divided by the volume occupied by one state.

Now it is the area it is a disc therefore, area between k t and k t plus d k t, what is the area? One fourth into 2 pi k t, d k t, 2 pi r, d r the area of the, so the area of this is 2 pi r d r, so 2 pi k t d k t, one fourth of it and of course, we need a factor to take care of the electron spin this is the in terms of area. Now we need to know the number of points which means what is the area occupied by 1 point in this case what do you think is the area occupied by 1 point please see corresponding to every value here and every value. Here there is a point, the next value here there is a point, next value here there is a point, so what do you have you have a square actually rectangle if L x is not equal to L y it is a rectangle, so you have a rectangle with the 4 points at the corner, but the every point is shared by 4 other rectangles so if I enlarge the view.

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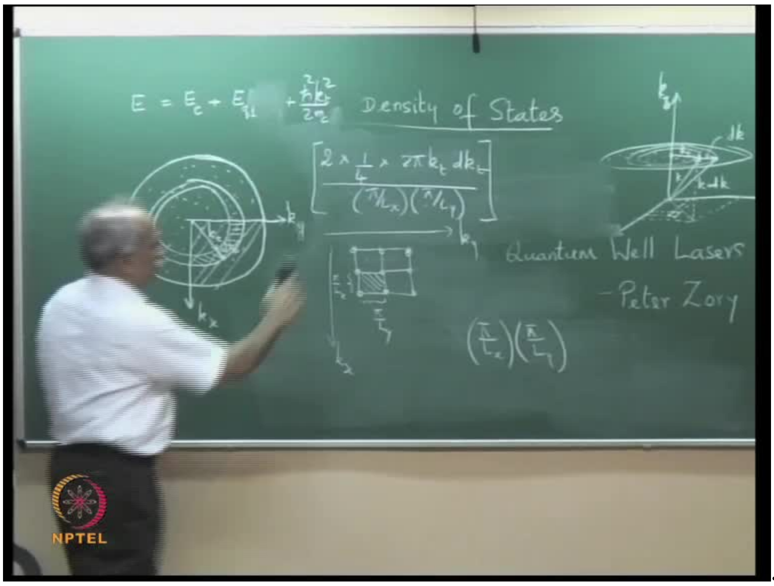

We have a situation, so we have points like, so this is x direction this is, so this is k x direction and this is k in the k space these points are here they are very closely packed points. I have just add 2 points, but actually if you zoom in then you will see that the points are sitting like this and what is disc separation pi by L x, what is this separation pi by L y. So the area of a rectangle here is pi by L x into pi by L y in the k space area of this rectangle where points represent k states allowed states, but you see that every point is surrounded by 4 such rectangles which means number of point per rectangle is one fourth one fourth because each contributes one fourth to this one fourth to this and one fourth to this like this. Therefore, the number of points per rectangle or area per point is pi by L x divided by pi by L y, area corresponding to one allowed state is this much in the k space the area in the first quadrant here is this divided by area corresponding to one state will give me number of states is this clear the area in the k space divided by area occupied by one state will give me number states.

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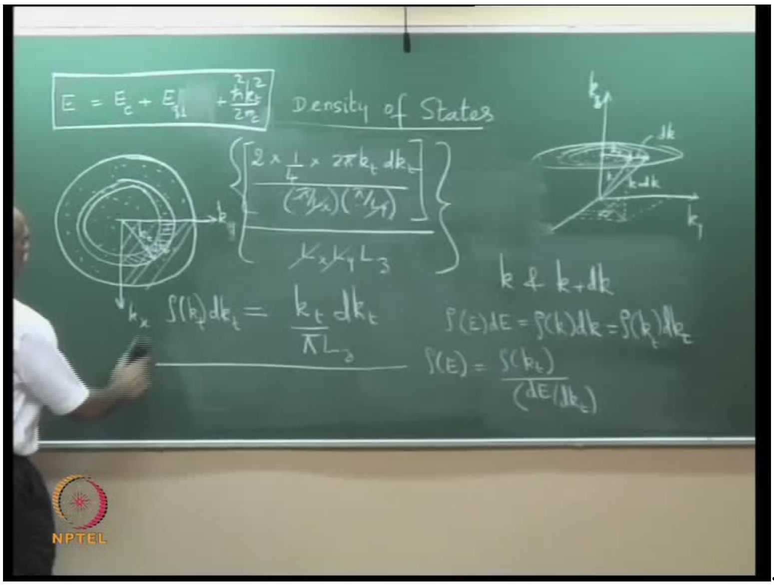

So, this divided by pi by L x into pi by L y this is the number of points between k and k plus d k, disc per unit volume of the material will give me density of states, so this what is the volume of the material L x into L y into L z, so this gives me the density of state. So please see it is just in one line or one expression the entire derivation is there 2 standing for the spin one fourth of the quadrant of area 2 pi k t d k t divided by area occupied by one state will give me the numerator gives me number of states between k t and d k t or k t k plus rho k plus k plus d k between k and k plus d k this is the number of points per unit volume that is the definition, so number of states per unit volume, so simplify this what will you get what do you get, so L x L y L z cancels.

And L z remains, so rho of k t, d k t equal to rho of k, d k is equal to k t, d k t, pi L z we see this you can cancel these though one pi goes here, so one pi remains in the denominator, L z remains in the denominator here, L z per unit volume, pi by L x divided by that is right, so in the k space we have got the density of states.

Now, as I indicated in the last class we would like to know the density of state in the E space then how do we go for E space we will use the expression relation between k t and E and use the fact that rho of E, d E is equal to rho of k, d k is equal to rho of k t ,d k t and therefore, rho of E finally, we need the density of states in the E space, so rho of E is equal to rho of k t divided by d E by d k t, I have used this equal to this and we have the expression for rho of k t already.

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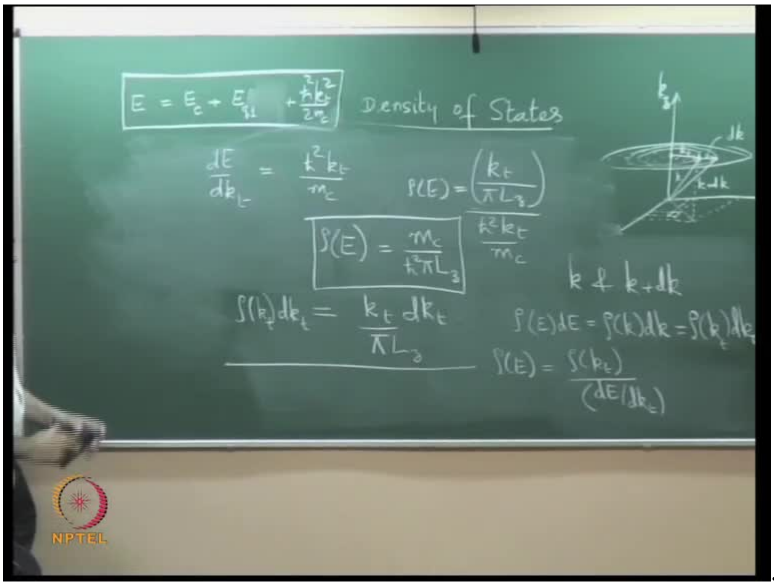

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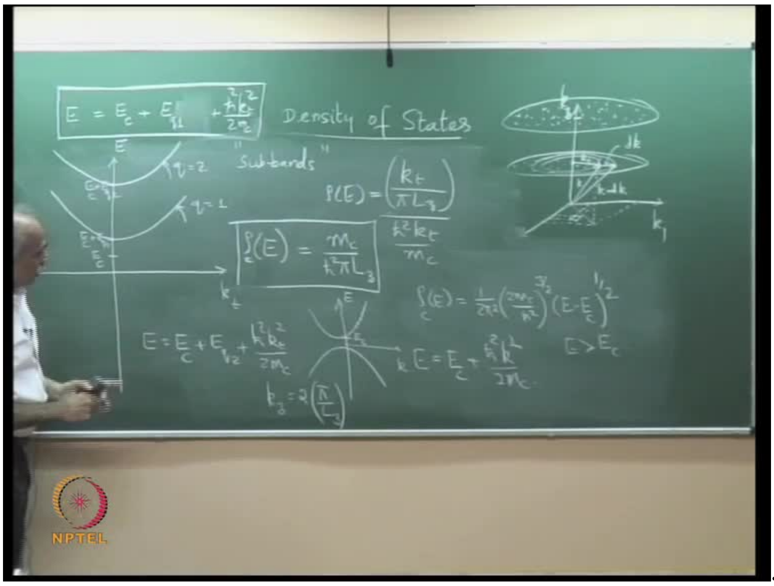

So if I may erase this, so if you have a clearer picture in one expression the entire derivation of the density of states is present. So d E by d k t let me do this simple algebra complete it, so d E by d k t. So this is a constant this is a constant for that plane this is a constant therefore, we simply will have h cross square into k t by m c 2, 2 cancels h cross square k t by m c this is d E by d k t, so rho of E therefore, is equal to rho of E is equal to rho of k t which is k t divided by pi into L z that divided by d E by d k t, so divided by h cross square k t, rho of k t divided by d E by d k t, h cross square k t divided by m c, so m c goes to the top, k t, k t cancels, so we have rho of E, Rho of E is equal to in a quantum well, rho of E is equal to m c divided by h cross square pi into L z where L z is the thickness of the quantum.

Something interesting that you see here that the density of states is independent of the energy right hand side there is no dependence on energy. Recall the density of state in a bulk rho c of E this is for the conduction band actually

Therefore this is also rho c, rho c of E is equal to 1 over 2 pi square, 2 m c by h cross square to the power E by 2 into E minus E c to the power half conduction band which means E for E greater than disc, there is a energy dependence, but there is no energy on the right hand side which means the density of state is constant, first point.

Now, let us come to some additional discussion about this energy, let us see what is this? This tells us that recall the E k diagram how did we have the E k diagram we had E, so E varying parabolically, so E here, so E was equal to E c plus h cross square k square divided by twice m c right from at k is equal to 0, so this is k here, E is equal to E c, so this is E c, what are these? These are simply nothing, but points of allowed states allowed states here, so you have large number of allowed states for k greater than 0, it is varying parabolically.

In this case you plot the density of states the E k diagram, k t versus E, up to E c you have no states, up to e c if you put k t equal to zero I have E c plus E q 1, E is equal to E, what is E? E is the allowed energy value of electrons. So this is E c the next level here is E c plus E q 1 beyond this as k t almost takes continuous values it varies parabolically in other words the band varies like this parabolically for q is equal to 1. We have now plotted with respect to k t not the total k with respect to k t, but what you need to see is earlier we had allowed states right from E c, now there are no states above E c up to E c plus E q 1 and your band starts from here, so this is a parabolic variation of the band what about when q is equal to 2 I have energy E is equal to E c plus E q 2 plus h cross square k t square by 2 m c, if I put q equal to 2 which means my k z is now 2 times pi by L z originally for q equal to 1, k z was pi by L z, now q equal to 2, 2 times pi by L z that value is suddenly a jump here, so this is E c plus E q 2 at E c equal to E q 2 I again have a parabolic variation, so we have the next sub band these are called energy sub bands, sub bands.

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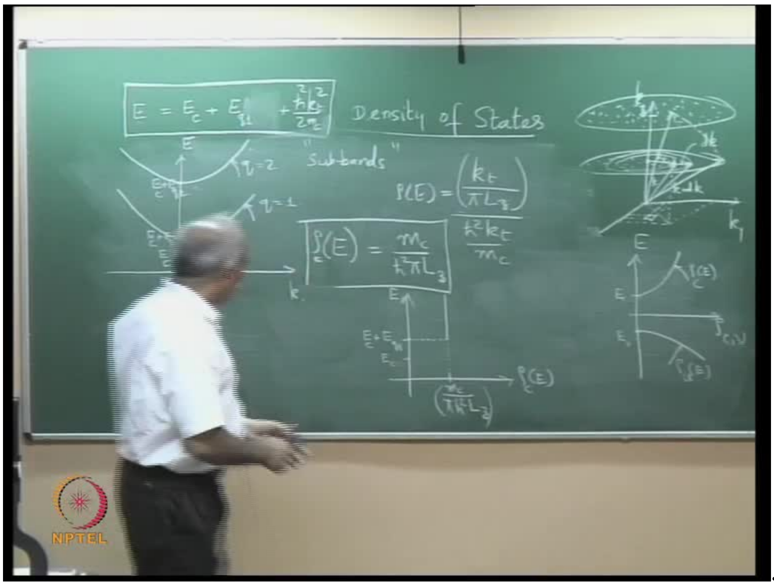

The E k diagram in a bulk has a parabolic variation here, in the case of a quantum well you have energy sub bands, these are bands because almost continuum k t takes almost continuous values because k x and k y take very large number of values, but k z has quantum jumps because pi by L z is a very large number because L z is a very small number. So it just jumps here for one value of k for this value of k you have large number of k x, k y values permitted next it goes to the next level and again large number of k x, k y values that is why in the case of quantum wells the energy band E k diagram is characterized by sub bands and corresponding to each sub band you have a density of states. Now why did I bring this here because if you see this, this was for q equal to 1 at q equal to 2, I have a second disc, now a second disc is available where again large number of points are present, if I change k energy changes, E changes if I have to plot this how would it look like let me first plot this rho of E you remember for the bulk I keep it here this is E and this is rho, rho of c comma v, we had E c, E minus E c square root dependence here.

So this was rho c of E we had shown this in the last class, so E c and similarly, for E v we had density of state varying like this where this variation is rho v of E we want to plot the corresponding variation here the density of states, let me show first only the conduction band at E is equal to E c we have no state because the first value of k starts E is equal to E q 1, So E q 1 that is E c plus E q 1, so this is E c plus E q 1, E q 1 is only that component h cross square, k z square by 2 m c, so E c plus E q 1 is the total energy at this value what is on this axis rho c of E. So up to this there were no density of states when we came here there is density of states and can you tell me what is the value here m c by m c divided by pi h cross square L z the density of states is constant this is the value what does that mean that means beyond E is equal to E c plus E q 1, we have density of state, but density of state is constant, density of state continuously increases with energy here, density of state is constant repeatedly I keep telling that why am I …

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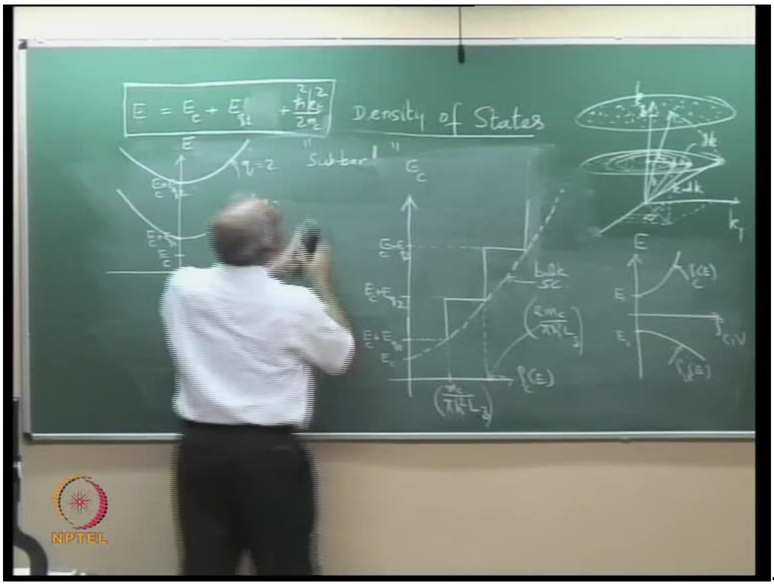

Density of state, so much many will think why after density of states for the last three class. Let me assure you that it is the density of states which will determine the device characteristics and the device performance. It is very important to understand the density of states, so its constant here what happens when energy as energy exceeds E c plus E q 2 we have a second sub band equivalently we have a second disc, so we have another amount of area that is if my k value becomes large. So let me show this k like this, this length is large if k is large, which means energy is large the tip of the vector can either lie in this disc or it can also lie E c the length is large it can also lie here, so when the energy is large you have the second disc available which means the density of state doubles the density of state for disc is what we have calculated here m c divided by pi h cross square into L z when you have a second disc available the density of states doubles and therefore, the density of states here for E, as E increases. That we continue on the same diagram E increases to E c plus E q 2 we have a second disk available and density of state simply jumps to this value.

What is this value here? 2 times m c by pi h cross square L z, so this value here is 2 m c by pi h cross square L z when you reach you can extend this E c plus E q 3, so E c plus E q 3 there is a third sub band available here which means there is a third disc available and you have the density of states making a third jump. What we have seen is this step like behavior in the density of states it so happen that if you draw the density of states my diagram is not very good. So what I have drawn here is the density of state corresponding to the bulk, bulk semi conductor this one if you draw the density of states corresponding to the bulk semi conductor you will get this step kind of variation. I leave this as an exercise to you to show that indeed in the bulk if you plot the density of state to quantum wells and bulk corresponding to E is equal to E c plus E q 1 the density of states that you get for the bulk is the same as this value. And if you put E c plus E q 2 in the expression for this you will get 2 times m c by pi h cross square L z.

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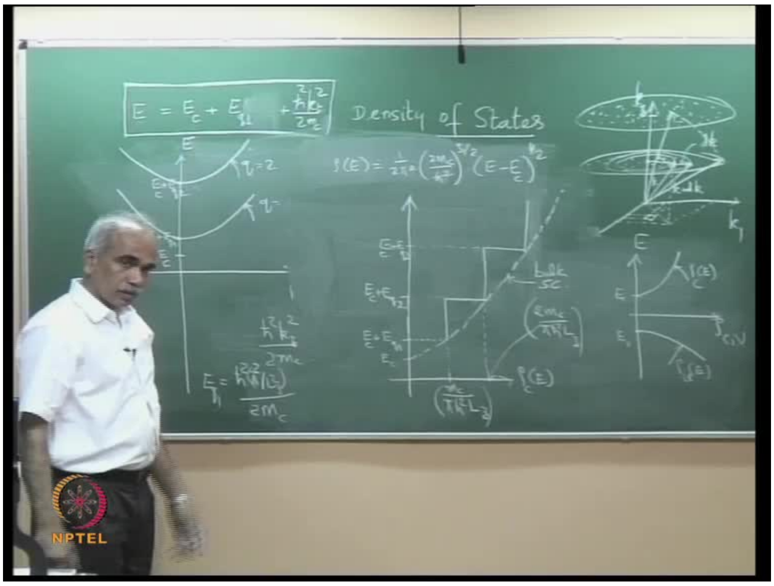

You just verify this which expression the expression for bulk where we have density of states rho of t is equal to 1 over 2 pi square into 2 m c by h cross square into 3 by 2 into E minus E c to the power half. If you substitute for E this value here you will get this result as this, if you substitute for E this value E c plus E q 2 means E c plus 4 pi square h cross square, so what is E q 2, E q 2 is h cross square E z square divided by twice m c, so E q 1 is equal to h cross square pi square by L z square divided by 2 m c, pi square by L z square divided by 2 m c, if you put E q 2 it will be 4 times because q equal to 2, so q square will become 4. So 4 times this if you substitute that value here you will get this number that is why the density of states is shown like that. Otherwise how do you know that this is touching this you substitute and see with indeed touches that value, so what we have seen is the density of states has a step like variation we will see its implications later when we go to the devices. My discussion has been focused only on the conduction band exactly similar discussion is applicable for the valance band and you will see the same step like behavior in the valance band.

So, let me give the final results for the density of states in a quantum well because the energy expression that I have written is for energy in the conduction band exactly similar discussion in the quantum in the valance band will give you similar results that I want to write the results.

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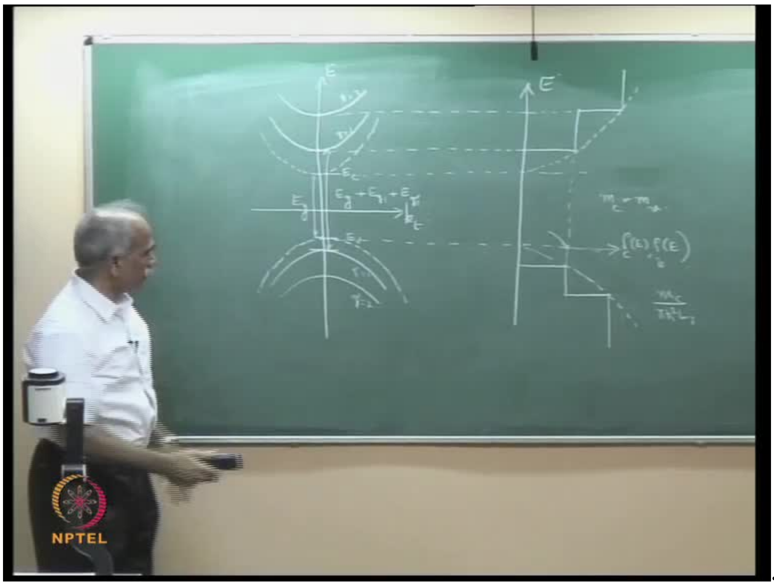

So, the E k diagram for a bulk t d L for a quantum well, so this is q dash equal to 1, q dash equal to 2, q dash is the corresponding number for the valance band, q equal to 1, q equal to 2 this is E k diagram. So E versus k t and here is E c and I have drawn this by dotted line because if you make a quantum well structure the first allowed states starts from here and immediate implication is the band gap of a semiconductor is E c minus E v this is E g if you make a quantum well structure the first allowed state is here and the first allowed whole state lowest energy whole is here the lowest the effective band gap is this that is original E g plus E q 1 plus E q dash 1, this is E q dash 1.

So what you see is by changing the structure into a quantum well structure you have effectively changed the band gap. We will discuss more about this later when we discuss about band gap engineering and we will discuss more about this, but this is the corresponding E k diagram and you have that corresponding density of states diagram. Everywhere vertical axis is E to the density of states for bulk and corresponding to, so we have this similar density of states, so this is rho c of E and rho E of E, so the dotted line corresponds to bulk and solid line corresponds to the quantum well structure. And I have assumed in showing that this point is the same as this point, I have assumed that m c equal to m v because recall that this value here was m c divided by pi h cross square into L z, if I am showing this value the same it means I have assumed m c equal to m v if m c is not equal to m v both the curvature here and the first the first value corresponding to the density of states would be different in the valance band which is in general to…

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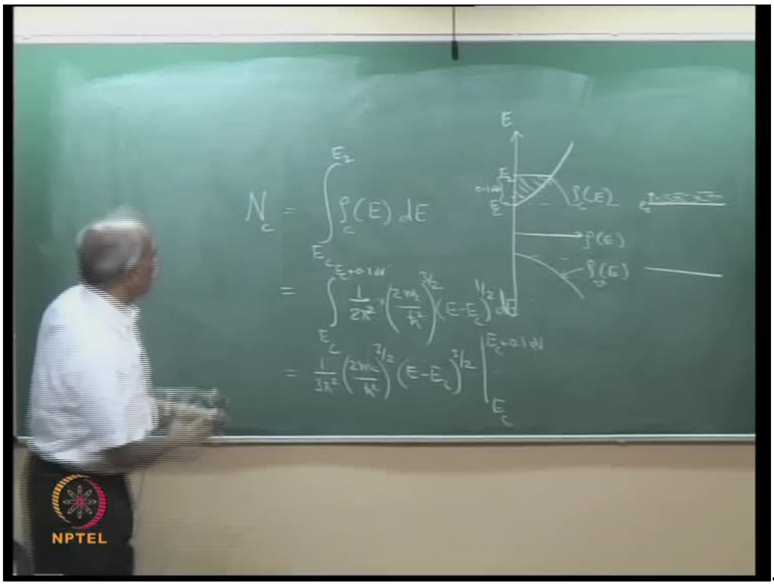

In general the density of states and the E k diagram variation is different in the valance, but if the effective masses are the same. Then they come at the same dilemma is this all right, we will discuss more about the quantum well and how to make etcetera at a later stage. So this is the E k diagram and this is E versus the density of stage why do we need density of states. Let us answer this question why do we need density of states because as I have already said that we want to know the carrier concentration, the carrier concentration is determined by the available states multiplied by the probability of occupation. How do we calculate the number of available states? The number of available states N is equal to rho c of E number of available states in the conduction band is equal to rho c of E d E integrate over E c to some value let us say up to some value E 2. You need the number of states up to E 2 what is this E 2, so E 2 I am plotting again this is E, this is rho of E rho c of E and rho v of E, this tells me the density of the states therefore, I want to calculate the actual number of states.

So, the number of states this is E c and I want to know up to some energy E 2. How many states are present here the dense the number of states is rho c of E, d E from E c to e 2, if you want to calculate the density of states in the entire band, so you write from E c up to the top of the band, so if you want to see up to some value e 2 substitute here and let us see what do we get, so this is equal E c for example, E 2 is equal to let us say this height is 0.1 E v let us put some numbers here. Now 0.1 E v I want to calculate from the you are familiar old band diagram which does not tell anything except energy gap, so if you want to calculate the density of state the number of states available here from E c this bottom up to some height how many states are available here. So I can calculate only through the density of states, so now we are coming to numbers. Let us see from E c up to this which means I calculate it from E c plus 0.1 E v substitute the values very quickly 1 over 2 pi square into twice m c by h cross square to the power 3 by 2 into E minus E c to the power half d E, integrate this what do you get this is constant.

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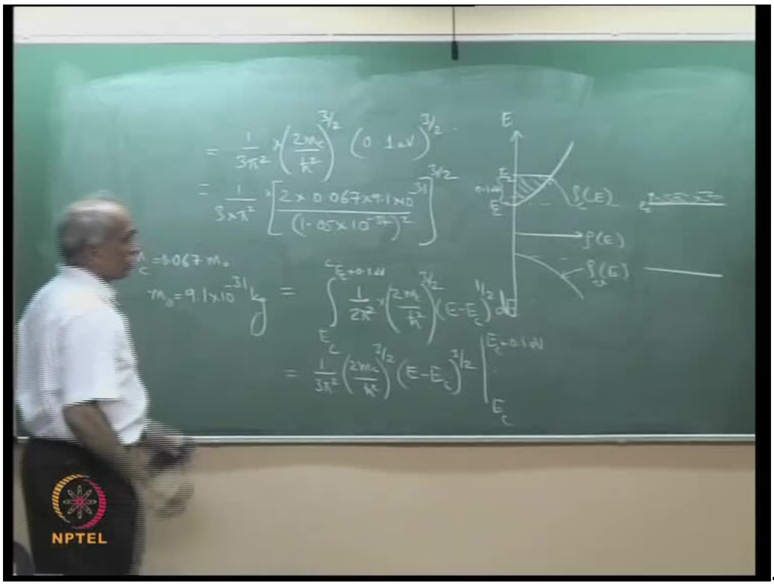

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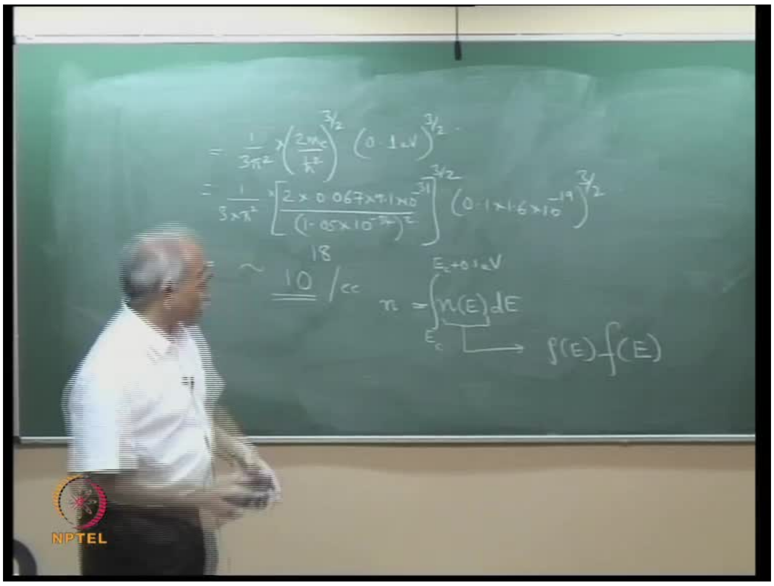

This is constant E minus E c to the power half integrate you get 3 by 2 and a factor 2 by 3 2 2 cancels, so you are left with 1 over 3 pi square into 2 m c by h cross square to the power of 3 by 2 into E minus E c to the power 3 by 2 from E c to E c plus 0.1 E v if you put E equal to E c it is 0, so it is simply E c plus 0.1 E v which means substitute the values 1 divided by 3 pi square into twice m c by h cross square to the power 3 by 2 into E minus E c is simply 0.1 E v the 0.1 E v to the power 3 by 2. So this is equal to 1 over 3 into pi square substitute value for pi into 2 into m c let us say gallium arsenate m c is equal to 0.67 times m 0 where m 0 equal to 9.1 into 10 to the power of minus 31 k g, so substitute m c equal to 0.067, 0.067 into 9.1 into 10 to the power of now you are like engineers calculate, this divided by h cross square h cross square is h, how much is h cross? 1.01 01 05.

Student: (( ))

05 all right.

So, 1.05 into 10 to the power of minus 34 h cross this is h cross, so h cross square and the whole to the power 3 by 2 into 0.1 E v it is in electron Volts whereas, all the others are s i units, so you have to convert this into Joules, so it is 0.1 into 1.6 into 10 to the power of minus 19 to the power 3 by 2, simplify this and find out what is the answer I think this will be of the order of 10 to the power of 18 the number is of the order of 10 to the power of 18 per cc, so we have find out how many states are available from the bottom of the conduction band up to some height 0.1 E v this is the available states, but if you want to know the carrier concentration then we have to have N of E, d E I want to get the carrier concentration N then it is N of E d b you integrate again from E c to E c plus 0.1 E v, but what is N of E density of carriers, carrier density? Carrier density is given by rho of E density of states multiplied by the probability of occupation.

The probability of occupation is given by the fermi function density of states multiplied by the probability. So now to know carrier concentration we need probability of occupation occupation probability. So this will be our next topic is occupation probability if I substitute the occupation probability multiplied by the density of states and you integrate you will get carrier concentration, now on we will get the numbers. So once the basic physics and the picture is clear then calculating numbers is not a problem at all, so our next topic will be probability of occupation, so I will stop here.